The Physical Model of the NIMROD Code

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EQUATIONS

Two Fluid:

$$n_i \cong n_e \equiv n$$

$$\frac{\partial n}{\partial t} + \frac{1}{e}\nabla \cdot \mathbf{J}_i = 0$$

$$\frac{\partial \mathbf{J}_i}{\partial t} + \nabla \cdot \frac{\mathbf{J}_i\mathbf{J}_i}{ne} = \frac{e}{m_i}\left(ne\mathbf{E} + \mathbf{J}_i \times \mathbf{B} - \nabla p_i - \nabla \cdot \Pi_i\right) - \frac{\eta n e^2}{m_i}\mathbf{J}$$

$$\frac{\partial \mathbf{J}_e}{\partial t} - \nabla \cdot \frac{\mathbf{J}_e\mathbf{J}_e}{ne} = \frac{e}{m_e}\left(ne\mathbf{E} - \mathbf{J}_e \times \mathbf{B} + \nabla p_e + \nabla \cdot \Pi_e\right) - \frac{\eta n e^2}{m_e}\mathbf{J}$$

$$\frac{3}{2}\left(\frac{\partial p_i}{\partial t} + \frac{\mathbf{J}_i}{ne} \cdot \nabla p_i\right) = -\frac{5}{2}p_i \nabla \cdot \left(\frac{\mathbf{J}_i}{ne}\right) - \nabla \cdot \mathbf{q}_i - \Pi_i : \nabla \cdot \left(\frac{\mathbf{J}_i}{ne}\right) + Q_i$$

$$\frac{3}{2}\left(\frac{\partial p_e}{\partial t} - \frac{\mathbf{J}_e}{ne} \cdot \nabla p_e\right) = \frac{5}{2}p_e \nabla \cdot \left(\frac{\mathbf{J}_e}{ne}\right) - \nabla \cdot \mathbf{q}_e + \Pi_e : \nabla \cdot \left(\frac{\mathbf{J}_e}{ne}\right) + Q_e$$

Maxwell's:

$$\mu_0 \mathbf{J} + \frac{1}{c^2}\frac{\partial \mathbf{E}}{\partial t} = \nabla \times \mathbf{B}$$

$$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E}$$

Neoclassical Closure:*

$$\Pi_s \cong \Pi_{s\parallel} = \left(\hat{\mathbf{b}}\hat{\mathbf{b}} - \frac{1}{3}\mathbf{I}\right)\left(p_\parallel - p_\perp\right)_s \text{ , s=i,e}$$

$$\left(p_\parallel - p_\perp\right)_s = -4 m_s n \mu_s \frac{\langle B^2 \rangle}{\left\langle \left(\hat{\mathbf{b}} \cdot \nabla B\right)^2 \right\rangle} \left(\mathbf{J}_s / n q_s \cdot \nabla\right) \mathit{ln} B$$

$$\mu_e \cong \frac{2.3 \varepsilon^{1/2} \nu_e}{\left(1 + 1.07 \nu_{*e}^{1/2} + 1.02 \nu_{*e}\right)\left(1 + 1.07 \varepsilon^{3/2} \nu_{*e}\right)}$$

$$\mu_i \cong \frac{0.66 \varepsilon^{1/2} \nu_i}{\left(1 + 1.03 \nu_{*i}^{1/2} + 0.31 \nu_{*i}\right)\left(1 + 0.66 \varepsilon^{3/2} \nu_{*i}\right)}$$

where

$\varepsilon = r / R$ and $\nu_{*s} \equiv \dfrac{\nu_s \varepsilon^{-3/2} q R}{v_{T_s}}$

*F. L. Hinton and R. D. Hazeltine, Rev. Mod. Phys. **48**, 239 (1976).

Particle 'closure':

The distribution function is split into drifting Maxwellian and perturbed parts.

$$f_s = \delta f_s + f_{s_M}$$

$$f_{s_M}(\mathbf{x},\mathbf{v},t) = \left(\frac{m_s}{2\pi k T_s(\mathbf{x},t)}\right)^{3/2} n_s(\mathbf{x},t)\, exp\left\{-\frac{m_s\left[\mathbf{v}-\mathbf{v}_s(\mathbf{x},t)\right]^2}{2kT_s(\mathbf{x},t)}\right\}$$

$$\frac{Df_s}{Dt} = \frac{D\delta f_s}{Dt} + \frac{Df_{s_M}}{Dt} = 0$$

$$\frac{D}{Dt} \equiv \frac{\partial}{\partial t} + \mathbf{v}\cdot\nabla_x + \frac{q_s}{m_s}(\mathbf{E}+\mathbf{v}\times\mathbf{B})\cdot\nabla_v$$

$$\frac{D}{Dt}\left(\frac{\delta f_s}{f_s}\right) = -\frac{1}{f_s}\frac{Df_{s_M}}{Dt} = -\left(1-\frac{\delta f_s}{f_s}\right)\frac{1}{f_{s_M}}\frac{Df_{s_M}}{Dt}$$

The evolution of the Maxwellian along a characteristic is determined by:

$$\frac{1}{f_{s_M}}\left(\frac{Df_{s_M}}{Dt}\right)_j = \frac{1}{T_s}\left(-\frac{5}{2}+\frac{m_s \mathbf{w}_j^2}{2kT_s}\right)\left(\mathbf{w}_j \cdot \nabla T_s\right)$$

$$+\frac{1}{n_s kT_s}\left(1-\frac{m_s \mathbf{w}_j^2}{3kT_s}\right)\left(\nabla \mathbf{v}_s : \Pi_s + \nabla \cdot \mathbf{q}_s\right)$$

$$-\frac{1}{n_s kT_s}\mathbf{w}_j \cdot \Pi_s + \frac{m_s}{kT_s}\mathbf{w}_j \cdot \left(\nabla \mathbf{v}_s \cdot \mathbf{w}_j - \frac{\mathbf{w}_j}{3}\nabla \cdot \mathbf{v}_s\right)$$

where $\mathbf{w}_j = \mathbf{v}_j - \mathbf{v}_s$, and $\mathbf{v}_j$ is the velocity of the j-th particle, and

$$\frac{D\mathbf{v}_j}{Dt} = \frac{q_s}{m_s}\left(\mathbf{E} + \mathbf{v}_j \times \mathbf{B}\right) .$$

The traceless stress tensor and heat flux are determined by:

$$\Pi_{s_g} = \frac{m_s \sigma}{\Delta V_g}\sum_j S\left(\mathbf{x}_g - \mathbf{x}_j\right)\left(\frac{\delta f_s}{f_s}\right)_j \left(\mathbf{w}_j \mathbf{w}_j - \frac{\mathbf{w}_j^2}{3} I\right)$$

$$\mathbf{q}_{s_g} = \frac{m_s \sigma}{2\Delta V_g}\sum_j S\left(\mathbf{x}_g - \mathbf{x}_j\right)\left(\frac{\delta f_s}{f_s}\right)_j \mathbf{w}_j \left(\mathbf{w}_j^2 - \frac{5kT_s}{m_s}\right),$$

where σ is a normalization such that

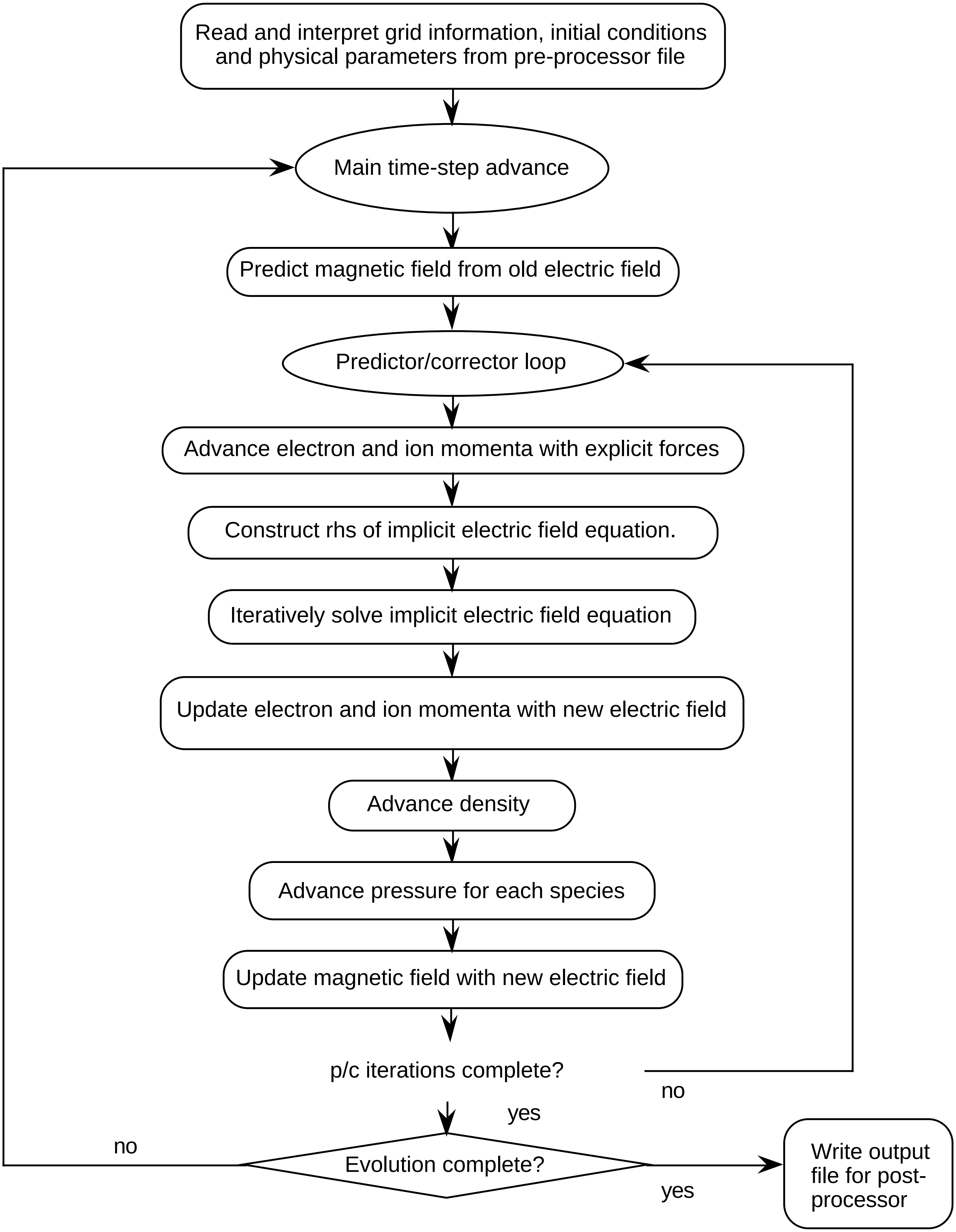
$$\sum_g n_{s_g} \Delta V_g = \sigma \sum_g \sum_j S\left(\mathbf{x}_g - \mathbf{x}_j\right).$$

NUMERICAL ALGORITHM

<u>Temporal Discretization:</u>

- Developed by D. Barnes, R. Nebel and D. Nystrom
- Used in PIC3D, TPCN and DMOM
  (finite difference)
- Abbreviated flowchart->

Abbreviated NIMROD Physics Algorithm Flowchart



At present, we advance the cold, collisionless fluid equations.

$$\frac{\mathbf{J}_s^{n+1} - \mathbf{J}_s^n}{\Delta t} = \frac{n_s q_s^2}{m_s}\mathbf{E} + \frac{f_\Omega q_s}{m_s}\mathbf{J}_s^{n+1} \times \mathbf{B} + \frac{(1 - f_\Omega) q_s}{m_s}\mathbf{J}_s^n \times \mathbf{B}$$

where f_Ω is a numerical time-centering parameter.

This leads to $\mathbf{J}_s^{n+1} = f(\mathbf{E})$:

$$\mathbf{J}_s^{n+1} = \left(1 - \frac{1}{f_\Omega}\right)\mathbf{J}_s^n + \mathbf{R}_s \cdot \left(\frac{1}{f_\Omega}\mathbf{J}_s^n + \frac{\Delta t n_s q_s^2}{m_s}\mathbf{E}\right)$$

where $\mathbf{R}_s = \dfrac{\mathbf{I} + \mathbf{r}_s \mathbf{r}_s - \mathbf{r}_s \times \mathbf{I}}{1 + r_s^2}$ and $\mathbf{r}_s = \dfrac{f_\Omega q_s \Delta t}{m_s}\mathbf{B}$.

Combining the species:

$$\frac{\Delta t}{\varepsilon_0}\mathbf{J}^{n+1} = \frac{\Delta t}{\varepsilon_0}\left(1 - \frac{1}{f_\Omega}\right)\mathbf{J}^n + \sum_s \mathbf{R}_s \cdot \frac{\Delta t}{\varepsilon_0 f_\Omega}\mathbf{J}_s^n + \mathbf{S} \cdot \mathbf{E}$$

where $\mathbf{S} = \sum_s (\omega_s \Delta t)^2 \mathbf{R}_s$.

In NIMROD, the algorithm was first implemented in the low-frequency (large Δt) limit, where $1 \ll r_i \ll r_e$ and

$$\mathbf{S} \rightarrow (\omega_e \Delta t)^2 \hat{\mathbf{b}}\hat{\mathbf{b}} + \frac{c^2}{f_\Omega^2 v_a^2}$$

and $\left(1 - \frac{1}{f_\Omega}\right)\mathbf{J}^n + \sum_s \mathbf{R}_s \cdot \frac{1}{f_\Omega}\mathbf{J}_s^n \rightarrow \mathbf{J}^n + \frac{1}{f_\Omega}\left(\hat{\mathbf{b}}\hat{\mathbf{b}} - \mathbf{I}\right)\cdot \mathbf{J}^n + \frac{\mathbf{M}^n \times \mathbf{B}}{f_\Omega^2 \Delta t B^2}$,

where **M** is the total momentum density.

We now have a run-time option to switch between 2-fluid and 'MHD.'

Combining the species equations with Ampere's law,

$\mu_0 \mathbf{J}^{n+1} = \nabla \times \nabla \times \mathbf{A}^{n+1}$, where $\frac{\mathbf{A}^{n+1} - \mathbf{A}^n}{\Delta t} = -\mathbf{E}$,

$$\mathbf{S} \cdot \mathbf{E} + (c\Delta t)^2 \nabla \times \nabla \times \mathbf{E} = \frac{\Delta t}{f_\Omega \varepsilon_0}\left(\mathbf{J}^n - \sum_s \mathbf{R}_s \cdot \mathbf{J}_s^n\right)$$

which is solved implicitly.

Thus, the present version of NIMROD advances the following set of equations:

$$\mathbf{A}^{+} = \mathbf{A}^{n} - \frac{\Delta t}{2}\mathbf{E}^{old}$$

$$\mathbf{B} = \nabla \times \mathbf{A}^{+}$$

$$\mathbf{S} \cdot \mathbf{E} + (c\Delta t)^2 \nabla \times \nabla \times \mathbf{E} = -\frac{\Delta t}{\varepsilon_0}\left[\mathbf{J}^{*}\right]$$

$$\mathbf{A}^{n+1} = \mathbf{A}^{n} - \Delta t\mathbf{E}$$

$$\mathbf{J}^{n+1} = \frac{1}{\mu_0}\nabla \times \nabla \times \mathbf{A}^{n+1}$$

$$\mathbf{M}^{n+1} = \mathbf{M}^{n} + \Delta t\left[f_{\Omega}\mathbf{J}^{n+1} + (1 - f_{\Omega})\mathbf{J}^{n}\right] \times \mathbf{B}$$

In the large Δt limit, with **B** fixed and **A** and **M** $\sim e^{i\mathbf{k}\cdot\mathbf{x}}$, the numerical dispersion relation is

$$\left\{(\lambda-1)^2+(kv_A\Delta t)^2\left[f_\Omega(\lambda-1)+1\right]^2\right\}$$
$$\times\left\{(\lambda-1)^2\left[1+\frac{(k_\perp v_A\Delta t)^2}{1+(\omega_e\Delta t)^2}\right]+\left(k_{||}v_A\Delta t\right)^2\left[f_\Omega(\lambda-1)+1\right]^2\right\}=0$$

where $\begin{pmatrix}\mathbf{A}\\ \mathbf{M}\end{pmatrix}^{n+1}=\lambda\begin{pmatrix}\mathbf{A}\\ \mathbf{M}\end{pmatrix}^{n}$.

The compressional wave comes from the first factor:

$$\lambda=1\pm ikv_A\Delta t\frac{1\pm if_\Omega kv_A\Delta t}{1+\left(f_\Omega kv_A\Delta t\right)^2}$$

Furthermore, $|\lambda|^2=1+\dfrac{(kv_A\Delta t)^2(1-2f_\Omega)}{1+\left(f_\Omega kv_A\Delta t\right)^2}$, so that for $1/2\le f_\Omega\le 1$, $|\lambda|\le 1$ for any Δt.

Spatial Discretization:

- Finite elements
- Block decomposition into
  -> structured blocks of logically rectangular cells
  -> unstructured regions of triangular cells
  -> sample tokamak grids
- Splined quantities are ‘scaled’ tensor components; for example, consider Ampere’s law (α’s are linear spline functions and g’s are metric elements):

$$\mu_0 \left(J^{(i)}\right)_a \sum_b \int J \alpha_a \alpha_b \, dxdy =$$

$$-\varepsilon^{ijk} \varepsilon^{mnp} \sum_b \left(A_{(p)}\right)_b \int \frac{g_{km}}{J} \frac{\partial\left(\alpha_a g_{ii}^{1/2}\right)}{\partial x^j} \frac{\partial\left(\alpha_b g_{pp}^{1/2}\right)}{\partial x^n} dxdy$$

where $J^{(i)} = (g_{ii})^{1/2} J^i$ is a ‘scaled contravariant’ or physical component and $A_{(p)} = \left(g_{pp}\right)^{-1/2} A_p$ is a ‘scaled covariant.’

-> separates parallel and perpendicular directions on field-aligned grids
-> preserves operator symmetry
-> avoids distortions due to nonuniform grid, which were encountered with ‘straight’ tensor representations

When spatial discretization is added to the numerical dispersion relation, we find terms which represent errors due to the finite element formulation.

Assume: $\mathbf{k} = k_x\hat{\mathbf{x}} + k_y\hat{\mathbf{y}}$, $\mathbf{B} = B_y\hat{\mathbf{y}} + B_z\hat{\mathbf{z}}$

$$\left\{(\lambda-1)^2\rho_x\rho_y - \left(\frac{v_A\Delta t}{\Delta x}\right)^2\left[f_\Omega(\lambda-1)+1\right]^2\left(\mathrm{K}_x\rho_y + \mathrm{K}_y\rho_x\, y^{-2}\right)\right\}$$

$$\times\left\{\begin{array}{l}\left[1+\dfrac{\left(\dfrac{v_A\Delta t}{\Delta x}\right)^2\left(\mathrm{K}_x\rho_y + \hat{b}_z^2\mathrm{K}_y\rho_x\, y^{-2}\right)}{\left[1+(\omega_e\Delta t)^2\right]\rho_x\rho_y}\right](\lambda-1)^2\rho_x\rho_y \\ -\left(\dfrac{v_A\Delta t}{\Delta x}\right)^2\hat{b}_y^2\mathrm{K}_y\rho_x\, y^{-2}\left[f_\Omega(\lambda-1)+1\right]^2\end{array}\right\}$$

$$= -\left(\frac{v_A\Delta t}{\Delta x}\right)^4\left[f_\Omega(\lambda-1)+1\right]^2 y^{-2}\left(\mathrm{K}_x\mathrm{K}_y\rho_x\rho_y - \kappa_x^2\kappa_y^2\right)$$

$$\times\left\{\hat{b}_z^2\left[f_\Omega(\lambda-1)+1\right]^2 + \frac{(\lambda-1)^2\hat{b}_y^2\rho_x\rho_y + \left(\dfrac{v_A\Delta t}{\Delta x}\right)^2\left[f_\Omega(\lambda-1)+1\right]^2\left(\mathrm{K}_x\rho_y + \mathrm{K}_y\rho_x\, y^{-2}\right)}{\left[1+(\omega_e\Delta t)^2\right]\rho_x\rho_y}\right\}$$

where

$$\mathrm{K}_j = 2\left[1-\cos\left(k_j\Delta j\right)\right] \leftrightarrow \left(k_j\Delta j\right)^2$$

$$\kappa_j = \sin\left(k_j\Delta j\right) \leftrightarrow k_j\Delta j$$

$$\rho_j = 1+\frac{\mathrm{K}_j}{6}$$

$$y = \frac{\Delta y}{\Delta x}$$